Lower and upper bounds on the fidelity susceptibility

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We derive upper and lower bounds on the fidelity susceptibility in terms of macroscopic thermodynamical quantities, like susceptibilities and thermal average values. The quality of the bounds is checked by the exact expressions for a single spin in an external magnetic field. Their usefulness is illustrated by two examples of many-particle models which are exactly solved in the thermodynamic limit: the Dicke superradiance model and the single impurity Kondo model. It is shown that as far as divergent behavior is considered, the fidelity susceptibility and the thermodynamic susceptibility are equivalent for a large class of models exhibiting critical behavior.

I. INTRODUCTION

Over the last decade there have been impressive theoretical advances concerning the concepts of entanglement and fidelity from quantum and information theory [1],[2],[3], and their application in condensed matter physics, especially in the theory of critical phenomena and phase transitions, for a review see [4, 5]. These two concepts are closely related to each other.

The entanglement measures the strength of non-local quantum correlations between partitions of a compound system. So it is natural to expect that entanglement will be a reliable indicator of a quantum critical point driven by quantum fluctuations. To this end the main efforts have been focused on the different entanglement measures and their behavior in the vicinity of the critical point [3–5].

The fidelity [6–9] naturally appears in quantum mechanics as the absolute value of the overlap (Hilbert-space scalar product) of two quantum states corresponding to different values of the control parameters. The corresponding finite-temperature extension, defined as a functional of two density matrices, ρ_1 and ρ_2,

$$\mathcal{F}(\rho_1, \rho_2) = \mathrm{Tr}\sqrt{\rho_1^{1/2}\rho_2\rho_1^{1/2}}, \tag{1}$$

was introduced by Uhlmann [6] and called fidelity by Jozsa [8]. Actually, the definition given by Jozsa, and used, e.g., by the authors of [10–13], is the square of $\mathcal{F}(\rho_1, \rho_2)$, however we shall adhere to the expression (1), as most authors do. This functional has become an issue of extensive investigations [14–18].

Closely related to the Uhlmann fidelity (1) is the Bures distance [19],

$$d_B(\rho_1, \rho_2) = \sqrt{2 - 2\mathcal{F}(\rho_1, \rho_2)} \tag{2}$$

which is a measure of the statistical distance between two density matrices. The Bures distance has the important properties of being Riemannian and monotone metric on the space of density matrices.

Being a measure of the similarity between quantum states, both pure or mixed, fidelity should decrease abruptly at a critical point, thus locating and characterizing the phase transition. Different finite-size scaling behaviors of the fidelity indicate different types of phase transitions [20]. The fidelity approach is basically a metric one [15] and has an advantage over the traditional Landau-Ginzburg theory, because it avoids possible difficulties in identifying the notions of order parameter, symmetry breaking, correlation length and so it is suitable for the study of different kinds of topological or Berezinskii-Kosterlitz-Thouless phase transitions.

Due to the geometric meaning of fidelity, the problem of similarity (closeness) between states can be readily translated in the language of information geometry [7, 21]. The strategy here is to make an identification of Hilbert-space geometry with the information-space geometry. Note that fidelity depends on two density matrices, ρ_1 and ρ_2, i.e. on the corresponding two points on the manifold of density matrices. On the other hand, being sensitive to the dissimilarity of states, it could be used to measure the loss of information encoded in quantum states.

The above mentioned decrease in the fidelity $\mathcal{F}(\rho_1, \rho_2)$, when the state ρ_2 approaches a quantum critical state ρ_1, is associated with a divergence of the fidelity susceptibility $\chi_F(\rho_1)$

[22] which reflects the singularity of $\mathcal{F}(\rho_1, \rho_2)$ at that point. The fidelity susceptibility $\chi_F(\rho_1)$, which is the main objects of this study, naturally arises as a leading-order term in the expansion of the fidelity for two infinitesimally close density matrices ρ_1 and $\rho_2 = \rho_1 + \delta\rho$. For simplicity, in our study we consider one-parameter family of Gibbs states

$$\rho(h) = [Z(h)]^{-1} \exp[-\beta H(h)], \tag{3}$$

defined on the family of Hamiltonians of the form

$$H(h) = T - hS, \tag{4}$$

where the Hermitian operators T and S do not commute in the general case, h is a real parameter, and $Z(h) = \mathrm{Tr} \exp[-\beta H(h)]$ is the corresponding partition function. Note that the fidelity and fidelity susceptibility under consideration are defined with respect to the parameter h, including the important symmetry breaking case when the system undergoes a phase transition as h is varied. The fidelity susceptibility at the point $h = 0$ in the parameter space is defined as (see e.g.[17]):

$$\chi_F(\rho(0)) := \lim_{h \to 0} \frac{-2 \ln \mathcal{F}(\rho(0), \rho(h))}{h^2} = - \left. \frac{\partial^2 \mathcal{F}(\rho(0), \rho(h))}{\partial h^2} \right|_{h=0}. \tag{5}$$

From (2) and (5) we obtain for the case of two infinitesimally close density matrices the following relation between the Bures distance and the fidelity susceptibility:

$$d_B^2(\rho(0), \rho(h)) = \chi_F(\rho(0))h^2 + O(h^4), \qquad h \to 0. \tag{6}$$

To avoid confusion, we warn the reader that for mixed states the definition of the fidelity susceptibility (5), based on the Uhlmann fidelity (1), differs from the one derived in [18] (see also [5]) by extending the ground-state Green's function representation to nonzero temperatures. This fact has been pointed out in [23], see also our Discussion.

The quantity (5) is more convenient for studying than the fidelity itself, because it depends on a single point $h = 0$ and does not depend on the difference in the parameters of the two quantum states [17, 24]. Physically, it is a measure of the fluctuations of the driving term introduced in the Hamiltonian through the parameter h. In the case when ρ_1 and ρ_2 commute, there are simple relations between the fidelity susceptibility (5) and thermal fluctuations. For examples, in the case of two states at infinitesimally close temperatures the fidelity susceptibility is proportional to the specific heat [16, 22]; in the case of spin systems

described by Hamiltonian of the form (4), with S being a projection of the total spin, then the fidelity susceptibility is proportional to the initial magnetic susceptibility [16, 17, 22]. In the non-commutative case, when the driving term does not commute with the Hamiltonian, such type of relation become more complicated.

It is our goal here to derive lower and upper bounds on theoretical information measures like fidelity susceptibility (5) and, therefrom, the Bures distance (6), in terms of thermodynamic quantities like susceptibility and thermal average values of some special observables. At that we concentrate on the most interesting non-commutative case.

The paper is organized as follows: in Section II we introduce our basic notations and derive an expression for the spectral representation of the fidelity susceptibility in the general noncommutative case, see (37), which is convenient for the derivation of inequalities involving macroscopic quantities, like susceptibilities and thermal average values. In Sections III and IV new upper, (40), and lower, (43), bounds on the fidelity susceptibility are derived. In Section V these bounds are checked against the exact expressions for the simplest case of a single quantum spin in an external magnetic field. We also consider the Kondo model (Section VI) and the Dicke model (Section VII) as non-trivial examples for testing our upper and lower bounds, and drawing conclusions about the behavior of the fidelity susceptibility itself. Finally, in Section VIII, we make some comments and compare our results to the inequalities derived in [18] for the Green's function based definition of fidelity susceptibility.

II.   FIDELITY SUSCEPTIBILITY

Here we consider the fidelity susceptibility (5) for the one-parameter family of Gibbs states (3) at the point $h = 0$. To this end we rewrite the density matrix (3) identically as

$$\rho(h) := \rho(0) + h\rho'(0) + (1/2)h^2\rho''(0) + r_3(h),$$

(7)

where

$$r_3(h) := \rho(h) - \rho(0) - h\rho'(0) - (1/2)h^2\rho''(0)$$

(8)

is expected to be of the order $O(h^3)$ as $h \to 0$. Next we calculate directly the derivatives in Eq. (7):

$$\rho'(0) = \rho(0)\beta \left[\int_0^1 S(\lambda)\mathrm{d}\lambda - \langle S \rangle_0 \right], \tag{9}$$

$$\rho''(0) = \rho(0)\beta^2 \left\{ \left[\int_0^1 S(\lambda)\mathrm{d}\lambda - \langle S \rangle_0 \right]^2 + \langle S \rangle_0^2 + \int_0^1 \mathrm{d}\lambda S(\lambda) \int_0^\lambda \mathrm{d}\lambda' S(\lambda') \right.$$
$$\left. - \int_0^1 \mathrm{d}\lambda \int_0^\lambda \mathrm{d}\lambda' S(\lambda - \lambda') S(\lambda) - \int_0^1 \mathrm{d}\lambda \langle S(\lambda) S \rangle_0 \right\}. \tag{10}$$

Here

$$S(\lambda) = \mathrm{e}^{\beta T \lambda} S \mathrm{e}^{-\beta T \lambda}, \tag{11}$$

and $\langle \dots \rangle_0$ denotes average value with the density matrix $\rho(0)$. For the further consideration it is important to note that, in conformity with the normalization conditions $\mathrm{Tr}\rho(h) = \mathrm{Tr}\rho(0) = 1$, we have

$$\mathrm{Tr}\rho'(0) = \mathrm{Tr}\rho''(0) = 0. \tag{12}$$

Our aim is to use the expansion (7) to calculate the square root in the definition of fidelity (1) with accuracy $O(h^2)$, as $h \to 0$, which is sufficient for obtaining the fidelity susceptibility, see Eq. (5).

To introduce our notation and for reader's convenience we derive here the matrix representation for the fidelity susceptibility in some detail. By using a slight extension of the method of [13], we set

$$\sqrt{\rho^{1/2}(0)\rho(h)\rho^{1/2}(0)} = \rho(0) + X + Y + Z, \tag{13}$$

where X, Y and Z are operators proportional to h, h^2 and h^3, respectively, to be defined below. By squaring Eq. (13), we obtain:

$$\rho^{1/2}\rho(h)\rho^{1/2} = \rho X + X\rho + X^2 + \rho Y + Y\rho + \rho Z + Z\rho + XY + YX + O(h^4). \tag{14}$$

Here and below, for brevity of notation we have set $\rho(0) = \rho$. Equating terms of the same order in h up to $O(h^3)$ yields a set of three equations:

$$h\rho^{1/2}\rho'(0)\rho^{1/2} = \rho X + X\rho, \tag{15}$$

$$(1/2)h^2\rho^{1/2}\rho''(0)\rho^{1/2} = X^2 + \rho Y + Y\rho, \tag{16}$$

$$\rho^{1/2}r_3(h)\rho^{1/2} = \rho Z + Z\rho + XY + YX. \tag{17}$$

To proceed with the calculations in the general case, when the operators T and S do not commute, we introduce a convenient spectral representation. To simplify the problem, we assume that the Hermitian operator T has a complete orthonormal set of eigenstates $|n\rangle$, $T|n\rangle = T_n|n\rangle$, where $n = 1, 2, \ldots$, with non-degenerate spectrum $\{T_n\}$. In this basis the zero-field density matrix $\rho(0)$ is diagonal too:

$$\langle m|\rho|n\rangle = \rho_m \delta_{m,n}, \qquad m, n = 1, 2, \ldots. \tag{18}$$

In terms of the matrix elements between eigenstates of the Hamiltonian T, Eq. (15) reads

$$h\rho_m^{1/2}\langle m|\rho'(0)|n\rangle\rho_n^{1/2} = (\rho_m + \rho_n)\langle m|X|n\rangle, \tag{19}$$

hence we obtain

$$\langle m|X|n\rangle = h\langle m|\rho'(0)|n\rangle\frac{\rho_m^{1/2}\rho_n^{1/2}}{\rho_m + \rho_n}. \tag{20}$$

Similarly, the second equation (16) yields

$$(1/2)h^2\rho_m^{1/2}\langle m|\rho''(0)|n\rangle\rho_n^{1/2} = \langle m|X^2|n\rangle + (\rho_m + \rho_n)\langle m|Y|n\rangle, \tag{21}$$

hence

$$\langle m|Y|n\rangle = -\frac{\langle m|X^2|n\rangle}{\rho_m + \rho_n} + (1/2)h^2\langle m|\rho''(0)|n\rangle\frac{\rho_m^{1/2}\rho_n^{1/2}}{\rho_m + \rho_n}. \tag{22}$$

Now we turn back to Eq. (13) and take the trace of both sides:

$$\mathrm{Tr}\sqrt{\rho^{1/2}(0)\rho(h)\rho^{1/2}(0)} = 1 + \mathrm{Tr}X + \mathrm{Tr}Y + \mathrm{Tr}Z. \tag{23}$$

In contrast to Ref. [13], no relationship between $\mathrm{Tr}X$ and $\mathrm{Tr}Y$ appears in our scheme. From Eq. (20) we obtain

$$\mathrm{Tr}X = (h/2)\mathrm{Tr}\rho'(0) = 0, \tag{24}$$

due to the explicit form of $\rho'(0)$, see (9). Next, taking into account Eq. (12) and the expressions (20), (22) for the matrix elements of X and Y, we calculate

$$\mathrm{Tr}Y = -\sum_{m,n}\frac{|\langle m|X|n\rangle|^2}{2\rho_m} + \frac{1}{4}h^2\mathrm{Tr}\rho''(0) = -\frac{1}{4}h^2\sum_{m,n}\frac{|\langle m|\rho'(0)|n\rangle|^2}{\rho_m + \rho_n}. \tag{25}$$

Thus, by substitution of the above results into (23), we derive with accuracy $O(h^2)$ the following expressions for the fidelity (1), where $\rho_1 = \rho(0)$ and $\rho_2 = \rho(h)$,

$$\mathcal{F}(\rho(0), \rho(h)) \simeq 1 - \frac{1}{4}h^2\sum_{m,n}\frac{|\langle m|\rho'(0)|n\rangle|^2}{\rho_m + \rho_n}, \tag{26}$$

and the squared infinitesimal Bures distance (6),

$$d_B^2(\rho(0), \rho(h)) \simeq \frac{1}{2} h^2 \sum_{m,n} \frac{|\langle m|\rho'(0)|n\rangle|^2}{\rho_m + \rho_n}. \tag{27}$$

Finally, the definition of (5) yields (see [13, 14, 18] for a similar matrix representation of the quantum fidelity susceptibility)

$$\chi_F(\rho) = \frac{1}{2} \sum_{m,n} \frac{|\langle m|\rho'(0)|n\rangle|^2}{\rho_m + \rho_n}. \tag{28}$$

Here matrix elements of $\rho'(0)$ are given by

$$\langle n|\rho'(0)|m\rangle = \frac{\rho_n - \rho_m}{T_m - T_n} \langle n|S|m\rangle, \qquad m \neq n, \tag{29}$$

and

$$\langle m|\rho'(0)|m\rangle = \rho_m \beta [\langle m|S|m\rangle - \langle S\rangle_0], \tag{30}$$

where

$$\langle S\rangle_0 := \sum_n \rho_n \langle n|S|n\rangle. \tag{31}$$

With the aid of the above expressions, the fidelity susceptibility (28) takes the form

$$\chi_F(\rho) = \frac{1}{2} \sum_{m,n,m\neq n} \left[\frac{\rho_n - \rho_m}{T_m - T_n}\right]^2 \frac{|\langle m|S|n\rangle|^2}{\rho_m + \rho_n} + \frac{1}{4}\beta^2 \langle (\delta S^d)^2\rangle_0, \tag{32}$$

where $\delta S^d = S^d - \langle S^d\rangle_0$, S^d being the diagonal part of the operator S:

$$S^d := \sum_m \langle m|S|m\rangle |m\rangle\langle m|. \tag{33}$$

Hence,

$$\langle (\delta S^d)^2\rangle_0 := \sum_m \rho_m \langle m|S|m\rangle^2 - \langle S\rangle_0^2. \tag{34}$$

Finally, by using the identity

$$\rho_m + \rho_n = (\rho_n - \rho_m) \coth X_{mn}, \tag{35}$$

where

$$X_{mn} \equiv \frac{\beta(T_m - T_n)}{2}, \tag{36}$$

we rewrite Eq. (32) in the form:

$$\chi_F(\rho) = \frac{\beta^2}{8} \sum_{m,n,m\neq n} \frac{\rho_n - \rho_m}{X_{mn}} \frac{|\langle n|S|m\rangle|^2}{X_{mn} \coth X_{mn}} + \frac{1}{4}\beta^2 \langle (\delta S^d)^2\rangle_0. \tag{37}$$

Here, the first term in the right-hand side describes the purely quantum contribution to the fidelity susceptibility, because it vanishes when the operators T and S commute, while the second term represents the "classical" contribution.

Now we are ready to derive lower and upper bounds on the fidelity susceptibility by applying elementary inequalities for $(x \coth x)^{-1}$ to the summand in the above expression.

III. UPPER BOUND

The application of the inequality $(x \coth x)^{-1} \leq 1$ to Eq. (37) readily gives:

$$\chi_F(\rho) \leq \frac{\beta^2}{8} \sum_{m,n,m \neq n} \frac{\rho_n - \rho_m}{X_{mn}} |\langle n|S|m \rangle|^2 + \frac{1}{4}\beta^2 \langle (\delta S^d)^2 \rangle_0. \tag{38}$$

By comparing the right-hand side to the expression for the Bogoliubov-Duhamel inner product (see, e.g., [25, 26] and references therein) of the self-adjoint operator δS with itself,

$$(\delta S; \delta S)_0 := \int_0^1 d\tau \langle \delta S(\tau) \delta S \rangle_0 = \frac{1}{2} \sum_{m,n,m \neq n} \frac{\rho_n - \rho_m}{X_{mn}} |\langle n|S|m \rangle|^2 + \langle (\delta S^d)^2 \rangle_0, \tag{39}$$

we obtain an upper bound in the transparent form

$$\chi_F(\rho) \leq \frac{\beta^2}{4} (\delta S; \delta S)_0. \tag{40}$$

Note that the right-hand side of the above inequality is priportional to the initial thermodynamic susceptibility:

$$(\delta S; \delta S)_0 = -\frac{N}{\beta} \frac{\partial^2 f[H(h)]}{\partial^2 h} \Big|_{h=0} := \frac{N}{\beta} \chi_N, \tag{41}$$

where $f[H(h)]$ is the free energy density of the system described by the Hamiltonian (4) and χ_N is the susceptibility with respect to the field h.

IV. LOWER BOUND

A lower bound follows by applying to the spectral representation for the fidelity susceptibility (37) the elementary inequality

$$(x \coth x)^{-1} \geq 1 - (1/3)x^2. \tag{42}$$

Then, from representation (37), we obtain the following lower bound for the fidelity susceptibility

$$\chi_F(\rho) \geq \frac{\beta^2}{4}(\delta S; \delta S)_0 - \frac{\beta^2}{24} \sum_{m,n,m\neq n} (\rho_n - \rho_m) X_{mn} |\langle n|S|m\rangle|^2$$

$$= \frac{\beta^2}{4}(\delta S; \delta S)_0 - \frac{\beta^3}{48}\langle [[S,T],S]\rangle_0. \tag{43}$$

V.   THE CASE OF A SINGLE SPIN IN MAGNETIC FIELD

To test the quality of the derived upper and lower bounds, we consider the simplest case of a single spin in external magnetic field subject to a transverse-field perturbation. By choosing the magnetic field in the reference state along the z-axis, and the transverse perturbation along the x-axis, the perturbed Hamiltonian takes the form

$$\beta H(h_1) = -h_1\sigma^x - h_3\sigma^z, \tag{44}$$

where σ^x and σ^z are the Pauli matrices. This choice corresponds to $\beta H(h_1)$ given by Eq. (4) with

$$\beta T = -h_3\sigma^z, \qquad \beta S = \sigma^x. \tag{45}$$

The fidelity (1) now measures the dissimilarities between the density matrices

$$\rho(h_1) = \frac{\exp\left(h_1\sigma^x + h_3\sigma^z\right)}{2\cosh\sqrt{h_1^2 + h_3^2}}, \tag{46}$$

and $\rho(0)$. The average values taken with the density matrix $\rho(0)$ will be denoted by the symbol $\langle\ldots\rangle_0$. Let $|1\rangle$ and $|-1\rangle$ be the eigenvectors of σ^z, as well as of the operator $\beta T = -h_3\sigma^z$: $\beta T|\pm 1\rangle = T_{\pm 1}|\pm 1\rangle$, where $T_{\pm 1} = \mp h_3$. Therefore, the density matrix $\rho(0)$ is diagonal in that basis and its nonzero matrix elements are

$$\rho_{\pm 1} := \langle\pm 1|\rho(0)|\pm 1\rangle = \frac{\exp(\pm h_3)}{2\cosh h_3}. \tag{47}$$

Next, for the first derivative (9) we have the expression

$$\rho'(0) := \frac{\partial}{\partial h_1}\rho(h_1, h_3)\bigg|_{h_1=0} = \rho \int_0^1 \sigma^x(\lambda)\mathrm{d}\lambda - \langle\sigma^x\rangle_0. \tag{48}$$

Taking into account that $\sigma^x|\pm 1\rangle = |\mp 1\rangle$, hence $\langle\sigma^x\rangle_0 = 0$, we obtain that

$$\langle\pm 1|\rho'(0)|\pm 1\rangle = 0, \qquad \langle\pm 1|\rho'(0)|\mp 1\rangle = \frac{\tanh h_3}{2h_3}. \tag{49}$$

Thus, for the fidelity susceptibility we obtain from Eq. (28) the following result

$$\chi_F(\rho) = \frac{|\langle -1|\rho'(0)|1\rangle|^2 + |\langle 1|\rho'(0)|-1\rangle|^2}{2(\rho_{-1} + \rho_1)} = \frac{\tanh^2 h_3}{4h_3^2}. \tag{50}$$

Evidently, the same result follows from expression (32), where the only nonzero matrix elements are $\langle -1|\beta S|1\rangle = \langle 1|\beta S|-1\rangle = 1$.

Let us check now the upper bound (40). First, by setting in (39) $\beta S = \sigma^x$ and $\beta \delta S = \sigma^x$, we obtain

$$\beta^2(\delta S; \delta S)_0 = \frac{\rho_{-1} - \rho_1}{T_1 - T_{-1}}|\langle -1|\beta S|1\rangle|^2 + \frac{\rho_1 - \rho_{-1}}{T_{-1} - T_1}|\langle 1|\beta S|-1\rangle|^2 = \frac{\tanh h_3}{h_3}. \tag{51}$$

Then, we note that $\beta S^d = 0$, hence

$$\chi_F(\rho) = \frac{\tanh^2 h_3}{4h_3^2} \leq \frac{\tanh h_3}{4h_3}, \tag{52}$$

which is equivalent to the initial inequality $(x \coth x)^{-1} \leq 1$.

Consider now the lower bound (43). An elementary calculation yields

$$\beta^3[[S,T],S] = -h_3[[\sigma^x, \sigma^z], \sigma^x] = 4h_3\sigma^z, \tag{53}$$

hence,

$$\beta^3\langle [[S,T],S]\rangle_0 = 4h_3 \tanh h_3, \tag{54}$$

and

$$\chi_F(\rho) \geq \frac{\tanh h_3}{4h_3}\left(1 - \frac{1}{3}h_3^2\right). \tag{55}$$

This lower bound amounts to initial elementary inequality (42) and it is always valid but makes sense for $h_3^2 < 3$ only.

VI.   APPLICATION TO THE KONDO MODEL

For a long time the Kondo model has been one of the challenging quantum many-body problems in condensed matter physics. Recent considerations have shown that solid state structures containing interacting spin systems (the Kondo model provides a specific example of such structures) are attractive candidates for quantum information processing [3].

In its simplest formulation, the effective Kondo Hamiltonian describes a single magnetic impurity spin interacting with a band of free electrons in a spatial domain Λ. The Hamiltonian has the form:

$$\mathcal{H}_\Lambda^K = H_0 - J(S_1 n^x + S_2 n^y + S_3 n^z), \tag{56}$$

where

$$H_0 = \sum_{k,\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma},$$

is the Hamiltonian for the conduction electrons. The fermion operator $c^\dagger_{k,\sigma}$ ($c_{k,\sigma}$) creates (annihilates) a conduction electron with momentum k and spin σ, J is the spin-exchange coupling between the magnetic impurity spin $\mathbf{S} = (S_1, S_2, S_3)$, $\mathbf{S}^2 = s(s+1)$, located at the origin $\mathbf{r} = 0$ and the conduction-electron spin densities, $\mathbf{n}(0) = (n^x, n^y, n^z)$ at $\mathbf{r} = 0$. In this case the Hilbert space naturally takes the form of a tensor product $\mathfrak{H} \otimes \mathbb{C}^{2s+1}$, where $\mathfrak{H}$ is the Hilbert space of the free electrons, and $\exp(-\beta \mathcal{H}^K_\Lambda)$ is of trace class and defines a Gibbs state [27].

Let us place the system in a homogeneous external field h in the direction of the z-axis,

$$\mathcal{H}^K_\Lambda(h) = \mathcal{H}^K_\Lambda - hS_3. \tag{57}$$

This choice corresponds to $H(h)$ given by (4) with

$$T := \mathcal{H}^K_\Lambda, \qquad S := S_3. \tag{58}$$

Due to the rotational invariance of the model Hamiltonian T, we have

$$\langle S_3 \rangle_0 = 0, \quad \langle S_3^2 \rangle_0 = (1/3)s(s+1), \tag{59}$$

where $\langle ... \rangle_0$ denotes average value with the density matrix

$$\rho(0) := \frac{e^{-\beta \mathcal{H}^K_\Lambda}}{\mathrm{Tr} e^{-\beta \mathcal{H}^K_\Lambda}}.$$

Now, our inequalities (40) and (43) yield the following bounds on the fidelity susceptibility.

$$\frac{\beta^2}{4}(S_3; S_3)_0 - \frac{\beta^3}{48}\langle [[S_3, T], S_3] \rangle_0 \leq \chi_F(\rho) \leq \frac{\beta^2}{4}(S_3; S_3)_0. \tag{60}$$

Here the double commutator and the Bogoliubov -Duhamel inner product in (60) can be estimated in terms of the model constants in (56) with the aid of the remarkable inequalities obtained by Röpstorff [28]:

$$1) \qquad 0 \leq \langle [[S_3, T], S_3] \rangle_0 \leq \frac{2}{3} J \tanh \beta J, \tag{61}$$

and

$$2) \qquad \chi_C \frac{1 - e^{-\beta\epsilon}}{\beta\epsilon} \leq \beta(S_3; S_3)_0 \leq \chi_C, \tag{62}$$

where χ_C is the Curie susceptibility (the initial susceptibility of a free spin)

$$\chi_C = \frac{\beta s(s+1)}{3}, \tag{63}$$

and the dimensionless quantity

$$\beta \epsilon = \frac{\beta J \tanh \beta J}{2s(s+1)}. \tag{64}$$

is introduced.

Let us use the Röpstorff's inequalities in combination with our inequalities. From (60), (61) and (62) we obtain the following bounds on the fidelity susceptibility

$$\chi_C \geq \frac{4}{\beta}\chi_F(\rho) \geq \chi_C \left[\frac{1 - \mathrm{e}^{-\epsilon\beta}}{\epsilon\beta} - \frac{1}{3}\epsilon\beta\right]. \tag{65}$$

These bounds can be readily analyzed and the formula exhibits some interesting properties. Since by definition $\chi_F(\rho)$ is a nonnegative function, the lowest meaningful bound in the left-hand side of (65) is zero. The upper bound gives the maximal possible value of $\chi_F(\rho)$. Note that $f(x) := (1 - e^{-x})/x$ is a strictly monotonically decreasing function of $x = [0, \infty)$, with $\lim_{x\to 0} f(x) = 1$ and $\lim_{x\to\infty} f(x) = 0$. As a result the equation

$$\frac{1 - \mathrm{e}^{-x}}{x} - \frac{1}{3}x = 0$$

has a unique solution $x = x^*$. Therefore, the lower bound in (65) is nonnegative in the interval $0 \leq \beta\epsilon \leq x^*$.

In the limit

$$\beta\epsilon = \frac{\beta J \tanh \beta J}{2s(s+1)} \to 0$$

we obtain an asymptotic relation between the fidelity susceptibility and Curie magnetic susceptibility (63)

$$\chi_F(\rho) \simeq \frac{\beta}{4}\chi_C. \tag{66}$$

From the previous consideration it is known that the above relation becomes equality if the driving term S and the Hamiltonian T commute, irrespectively of the concrete model. Indeed, this is the case in the Kondo problem in the classical limit of infinite spin, $s \to \infty$, with β held fixed. Another possibility (66) to take place asymptotically is $\beta J \to 0$. Note that, in the case $\infty > \beta\epsilon > x^*$, where the lower positive bound follows from the definition of $\chi_F(\rho)$, we obtain the inequalities

$$0 < \chi_F(\rho) \leq \frac{\beta}{4}\chi_C. \tag{67}$$

between the fidelity susceptibility and Curie magnetic susceptibility (63).

In general, we see that $(4/\beta)\chi_F(\rho)$ can be smaller than the free spin susceptibility but exceeds some nonnegative value given by

$$\max\left[\frac{1-e^{-\epsilon\beta}}{\epsilon\beta} - \frac{1}{3}\epsilon\beta, \quad 0\right],$$

which depends on the parameter $\beta\epsilon$.

If $\beta\epsilon$ is close to zero then $(4/\beta)\chi_F(\rho)$ is close to the free spin susceptibility. In other words, from the bounds obtained here it is seen that, when $\beta\epsilon \to 0$, as well as when $s \to \infty$, the deviation of $(4/\beta)\chi_F(\rho)$ from the single-spin Curie law tends to zero.

VII. APPLICATION TO THE DICKE MODEL

The Dicke model [29] considers the interaction between N two-level atoms and the quantized single-mode electromagnetic field in a cavity Λ of volume V. Working at a constant density $n = N/V$, one can take the Hamiltonian in the form

$$\mathcal{H}_N^D = \omega a^+ a + \epsilon J_N^z + \lambda N^{-1/2}(a+a^+)J_N^x. \tag{68}$$

Here a and a^+ denote the annihilation and creation operators for the cavity mode with frequency $0 < \omega < \infty$ which act on the one-mode Fock space $\mathcal{F}_B$ and satisfy the commutation relations $[a^+, a^+] = [a^-, a^-] = 0, [a^+, a^-] = 1$; $J_N^\alpha = (1/2)\sum_{i=1}^N \sigma_i^\alpha$, where σ^α ($\alpha = x, y, z$) are the Pauli matrices acting on a two dimensional complex Hilbert space $\mathcal{C}^2$, describe the ensemble of two-level atoms, the real ϵ is the atomic level splitting and $0 < \lambda < \infty$ is the coupling strength of the atom-field interaction.

With the aid of different methods, it was rigorously proven that in the thermodynamic limit the Dicke model exhibits a second order phase transition from a normal to a superradiant phase [30–32]. For values of the parameters λ, ω and ϵ obeying the condition $4\lambda^2/\omega < |\epsilon|$, no phase transition occurs at any temperature, whereas for $4\lambda^2/\omega > |\epsilon|$ there exists a finite critical temperature $T_c = (|\epsilon|/2)\tanh(|\epsilon|\omega/4\lambda^2)$. At the point $T = 0$, $4\lambda^2/\omega = |\epsilon|$, the model exhibits another, quantum phase transition of second order driven by the parameter λ . Quite recently, a renewed interest to this issue appeared due to studies of quantum entanglament. The superradiant quantum phase transition at the critical point $\lambda_c = \sqrt{|\epsilon|\omega}/2$ manifests itself, among other phenomena, in the entanglement between the atomic ensemble and the field mode.

Let us introduce a source term S for the electromagnetic field in the form

$$\mathcal{H}_N^D(h) = \mathcal{H}_N^D - hS, \quad S := \sqrt{N}(a^+ + a)/2,$$

where h is a real field conjugate to the self-adjoint operator S. Then, the second derivative of the corresponding free energy density with respect to h is

$$\frac{\partial^2 f[\mathcal{H}_N^D(h)]}{\partial^2 h} = -\beta(\delta S; \delta S)_{\mathcal{H}_N(h)}, \tag{69}$$

where $\delta S := S - \langle S \rangle_{\mathcal{H}_N^D(h)}$. Let us note that in the thermodynamic limit the second derivative diverges at the point $(h = 0, \quad T = T_c)$.

In the case under consideration our inequalities (40) and (43) yield

$$\frac{\beta^2}{4}(\delta S; \delta S)_0 - \frac{\beta^3}{48}\langle[[S, \mathcal{H}_N^D], S]\rangle_0 \leq \chi_F(\rho) \leq \frac{\beta^2}{4}(\delta S; \delta S)_0,$$

where the subscript "0" is used instead of the Hamiltonian $\mathcal{H}_N^D$. One readily calculates

$$\langle[[S, \mathcal{H}_N^D], S]\rangle_0 = N\omega, \tag{70}$$

and, by using the definition (41) of the initial susceptibility per particle with respect to the driving field h, we obtain the bounds

$$\frac{\beta}{4}\chi_N - \frac{\beta^3\omega}{48} \leq \frac{\chi_F(\rho)}{N} \leq \frac{\beta}{4}\chi_N.$$

Using these inequalities one can estimate apart the classical contribution and the quantum contribution to the fidelity susceptibility. When the size of the system increases $N \to \infty$ at the critical temperature T_c, the thermodynamic susceptibility $\chi_N \to \infty$ and for a fixed value of $\beta\omega/48$ we have the asymptotical result

$$\frac{\chi_F(\rho)}{N} \simeq \frac{\beta}{4}\chi_N.$$

Such a relation is a feature of classical systems. The above relation should be exact if $\mathcal{H}_N^D$ and S commute, which is not the case. However, one can state that due to the strong classical fluctuations there is a temperature region around T_c with borders defined by the condition

$$\beta_c^{-1}\chi_N \gg \frac{\beta_c\omega}{12},$$

where the influence of the quantum fluctuations on the relationship between χ_N and $\chi_{F(\rho)}/N$ is suppressed.

VIII. DISCUSSION

The study of theoretical information properties of quantum models at the critical point is a hot topic of a primary interest in the last decade. First, it allows one to explore the quantum world as a resource in quantum information processing. Second, it sheds light on the critical phenomena from a different point of view, being an useful tool in the case when the standard Landau-Ginzburg approach based on the idea of symmetry breaking is hampered. As a result, the obtained so far knowledge opens an exciting possibility of the study in a unified framework of quantum information theory, critical phenomena paradigms, and novel quantum phases of matter. Our consideration is an additional step in this direction.

Let us mention that important results on the role of critical fluctuations in systems with broken symmetries have been obtained in the past using famous inequalities due to Bogoliubov, Mermin-Wagner, Griffits, among others, see, e.g. [25, 33–35]. It should be stressed that a noteworthy property of this inequality approach is that the obtained results are exact and cannot be inferred from any perturbation theory. The benefits of having exact statements about strongly interacting systems are difficult to overestimate. A survey of some other inequalities, used to solve problems arising in the Approximating Hamiltonian Method, has been recently given in [26] along with a number of references.

Inequalities, as a tool for obtaining interesting exact statements, are also wide-spread and traditional in the information theory, see e.g.[11, 36, 37].

Our lower (43) and upper (40) bounds indicate that for the detection of phase transitions between mixed states the fidelity susceptibility per particle χ_F/N is as efficient as the usual susceptibility χ. This conclusion is in conformity with the commonly accepted view that quantum fluctuations are dominated by the thermal ones when $T_c > 0$. However, one should keep in mind that our results were derived under rather restrictive conditions on the spectrum of the Hamiltonian.

The same conclusion has been drawn in [18], although for a different definition of the fidelity susceptibility. A number of authors, see e.g. [5, 18], start from the expansion of the zero-temperature definition of fidelity (at $\beta = \infty$)

$$|\langle\psi_0(h)||\psi_0(0)\rangle| \simeq 1 - \frac{1}{2}h^2\chi_F(\infty), \quad h \to 0, \tag{71}$$

where $\psi_0(h)$ is the ground state eigenfunction of Hamiltonian (4). In terms of the spectral

representation of the operator $H(0) = T$, this yields [21, 22]:

$$\chi_F(\infty) = \sum_{n \neq 0} \frac{|\langle \psi_n(0)|S|\psi_0(0)\rangle|^2}{[T_n - T_0]^2}. \tag{72}$$

This quantity is related to the imaginary-time correlation function

$$G(S|\tau) = \theta(\tau)[\langle S(\tau)S\rangle_0 - \langle S\rangle_0^2], \tag{73}$$

where θ is the Heaviside step function, as follows [21, 22]:

$$\chi_F^G(\infty) = \int_0^\infty \tau G(S|\tau)d\tau. \tag{74}$$

Its finite-temperature generalization is defined as [18, 38]

$$\chi_F^G(\beta) = \int_0^{\beta/2} \tau G(S|\tau)d\tau, \tag{75}$$

where $G(S|\tau)$ is again given by (73) but the symbol $\langle ... \rangle_0$ now denotes the thermal average in the Gibbs ensemble with Hamiltonian $H(0) = T$. A subtle point in this definition is the upper integration limit $\beta/2$, in lieu of β, which was justified by path-integral arguments and a Quantum Monte Carlo method in [18].

In Ref. [23] it was found that definition (75) of the fidelity susceptibility $\chi_F^G(\beta)$ is based on a definition of the fidelity itself,

$$F^G(\rho_1, \rho_2) = \text{Tr}\sqrt{\rho_1^{1/2}\rho_2^{1/2}}, \tag{76}$$

which is different from Uhlmann's definition (1) that was accepted in the present study.

Let us consider the bounds on $\chi_F^G(\beta)$ obtained in [18]:

$$\frac{1}{2}ds^2(0, \beta) \leq \chi_F^G(\beta) \leq ds^2(0, \beta), \tag{77}$$

where (in our notation)

$$ds^2(0, \beta) = \frac{1}{4}\beta^2\langle(\delta S^d)^2\rangle_0 + \sum_{n>m} \frac{|\langle m|S|n\rangle|^2}{(T_m - T_n)^2}\,\rho_n\frac{\left(1 - e^{-2X_{mn}}\right)^2}{1 + e^{-2X_{mn}}} \tag{78}$$

Here $ds^2(0, \beta)h^2$ is the leading-order term in the expansion of the squared Bures distance between the states $\rho(0)$ and $\rho(h)$ as $h \to 0$. As expected from relation (6), expression (78) exactly equals our fidelity susceptibility $\chi_F(\rho)$, as given by spectral representation (32). Thus, inequalities (77) provide a new lower bound on $\chi_F(\rho)$,

$$\chi_F(\rho) \geq \chi_F^G(\beta), \tag{79}$$

which is a kind of dynamical structural factor of the driving Hamiltonian S. An advantage of this bound is that it can be computed with the aid of the quantum Monte Carlo stochastic series expansion [38]. From the spectral representation of [18]

$$\chi_F(\rho) \geq \chi_F^G(\beta) = \frac{1}{8}\beta^2 \langle (\delta S^d)^2 \rangle_0 + \sum_{n>m} \frac{|\langle m|S|n \rangle|^2}{(T_m - T_n)^2} \left(\sqrt{\rho_m} - \sqrt{\rho_n}\right)^2, \tag{80}$$

we conclude that the lower bound (79) follows from expression (32) and the elementary inequality

$$(\rho_n - \rho_m)^2 \geq (\rho_n + \rho_m)(\sqrt{\rho_m} - \sqrt{\rho_n})^2.$$

At that, the resulting bound will be with the better coefficient $1/4$ of the classical term instead of $1/8$ as in (80).

We have established bounds on the fidelity susceptibility which are expressed in terms of thermodynamic quantities. An additional reasoning that stimulates this line of consideration of information-theoretic quantities, is that the experimental setup for measuring thermodynamic quantities is well developed. Thus, estimation of metric quantities with a thermodynamic-based experiment seems to be very appealing. We have shown that as far as divergent behavior in the thermodynamic limit is considered, the fidelity susceptibility χ_F and the usual thermodynamic susceptibility χ are equivalent for a large class of models exhibiting critical behavior. It remains for the future to study the effect of degeneracy, especially macroscopic one, of the ground state on the upper and lower bounds for the fidelity susceptibility.

Acknowledgements

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